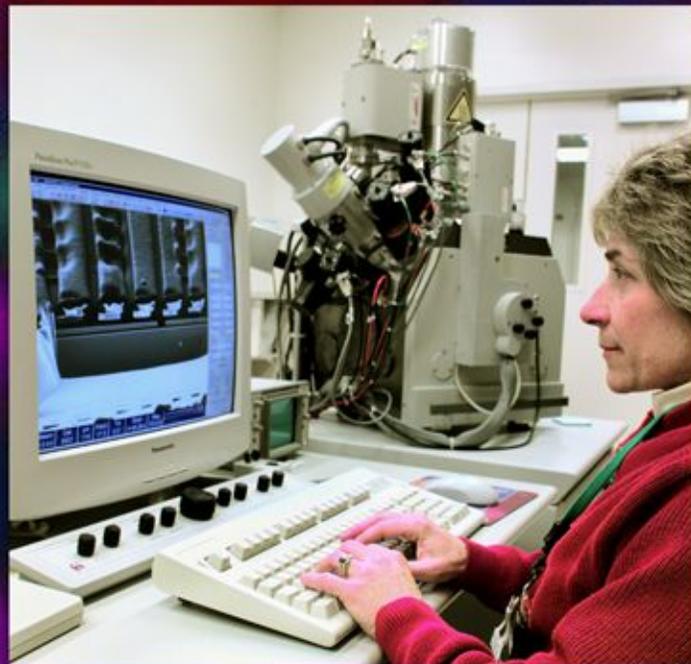


WINTER • 2000-2001



A QUARTERLY RESEARCH & DEVELOPMENT JOURNAL
VOLUME 2, NO. 4

A MATERIAL WORLD Tailoring Materials for the Future



ALSO:

**New Materials for Microsystems
Predictive Modeling Meets the Challenge**



**Sandia
National
Laboratories**

A Department of Energy
National Laboratory



Officials of FIRCO and CONAE (the Mexican National Commission for Energy Savings) discuss the recent installation of Sandia's photovoltaic water-pumping station on Rancho Sagitario in Baja California Sur, just outside of La Paz, Mexico. The ranch manager is standing in the background (in the hat). (From left: Oscar Sandoval, Regional Director of CONAE in Chihuahua; ranch manager, name not known; Jesús Parada, FIRCO, Chihuahua; and Simón Ortiz, FIRCO, Baja California Sur.)

ON THE COVER:

Bonnie Mckenzie operates a dual beam Focused Ion Beam/Scanning Electron Microscope (FIB/SEM). The image on the computer screen shows a cross section of a radiation-hardened device. The cross section was rendered with the FIB/SEM and allowed the observation of stress voids that could result in device failure. The background image is a spectrum image of a two-phase steel taken in a Scanning Electron Microscope. The image was analyzed using Sandia's newly developed information-extraction software.

Sandia Technology is a quarterly journal published by Sandia National Laboratories. Sandia is a multiprogram engineering and science laboratory operated by Sandia Corporation, a Lockheed Martin company, for the Department of Energy. With main facilities in Albuquerque, New Mexico, and Livermore, California, Sandia has broad-based research and development responsibilities for nuclear weapons, arms control, energy, the environment, economic competitiveness, and other areas of importance to the needs of the nation. The Laboratories' principal mission is to support national defense policies, by ensuring that the nuclear weapon stockpile meets the highest standards of safety, reliability, security, use control, and military performance. For more information on Sandia, see our Web site at <http://www.sandia.gov>.

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FROM THE *Editor*

Dear Readers:

Materials science—always a vital research area at Sandia National Laboratories—is taking on even greater importance as the nation’s nuclear weapons stockpile ages. Materials science is the study of the properties of solid materials and how those properties are determined by a material’s composition and structure. Materials science can’t be understood within the context of any single discipline and therefore combines an amalgam of many fields including solid-state physics, metallurgy, and chemistry. By understanding the origins of properties, materials can be selected or designed for an enormous variety of applications, ranging from steel and lightweight polymer components to silicon for the manufacture of integrated circuits and microsystems.

Sandia’s work in materials science is critical to stockpile stewardship, or ensuring our nation’s aging nuclear arsenal remains safe, secure, and reliable. The nuclear arsenal is getting older than its design life, and with nuclear testing suspended, we must rely on fundamental science to ensure weapon components will continue to function and yet remain safe and secure as they remain in the stockpile.

Sandia’s research in materials science continues to break new ground, particularly as we broach the relatively new areas of nano- and biotechnology. What has become immediately appreciable is that much of our work in materials science—while focused on the weapons program—has applications in many different areas that will benefit Americans for years to come.

Chris Miller
Editor

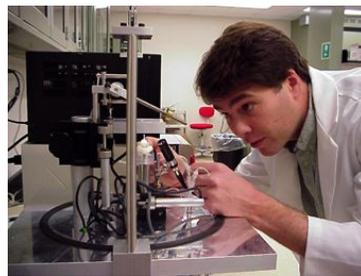
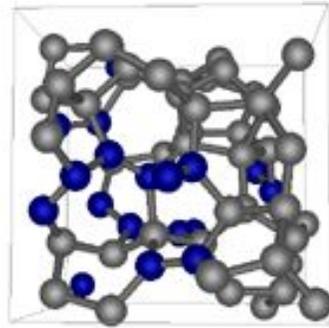


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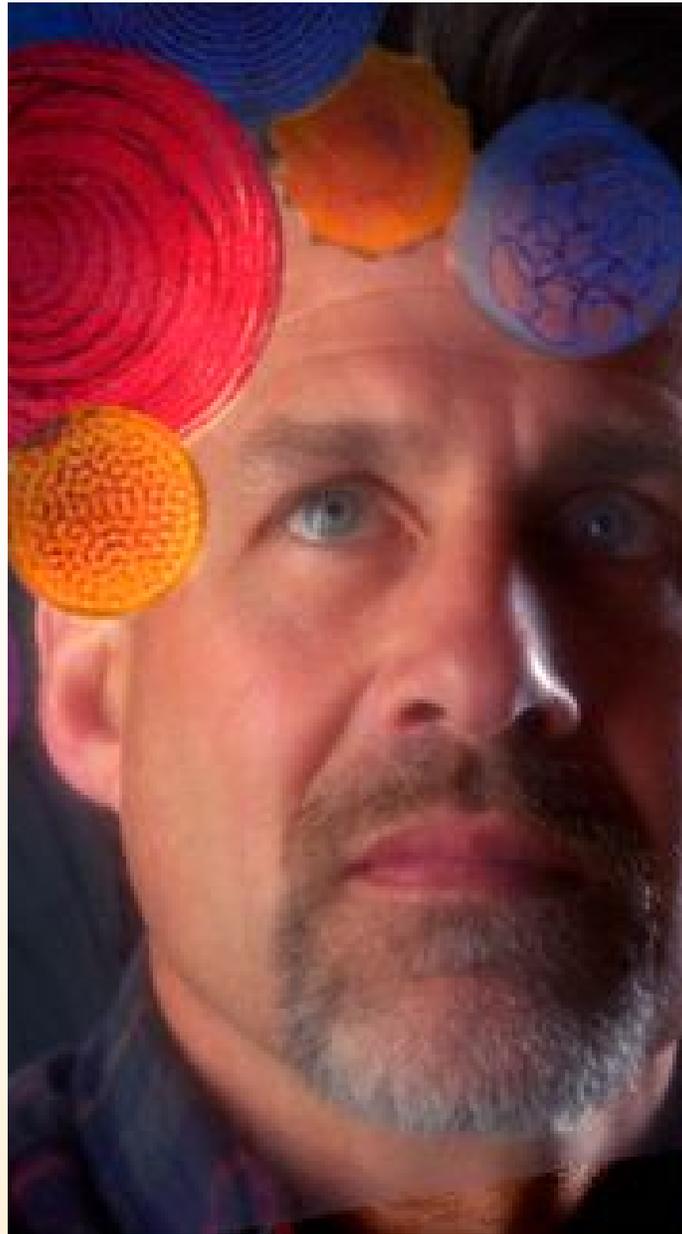
INSIGHTS

By V.S. Arunachalam, Distinguished Service Professor in the Department of Materials Science & Engineering, Engineering & Public Policy, and The Robotics Institute of Carnegie Mellon University in Pittsburgh, Pennsylvania.

A Material World

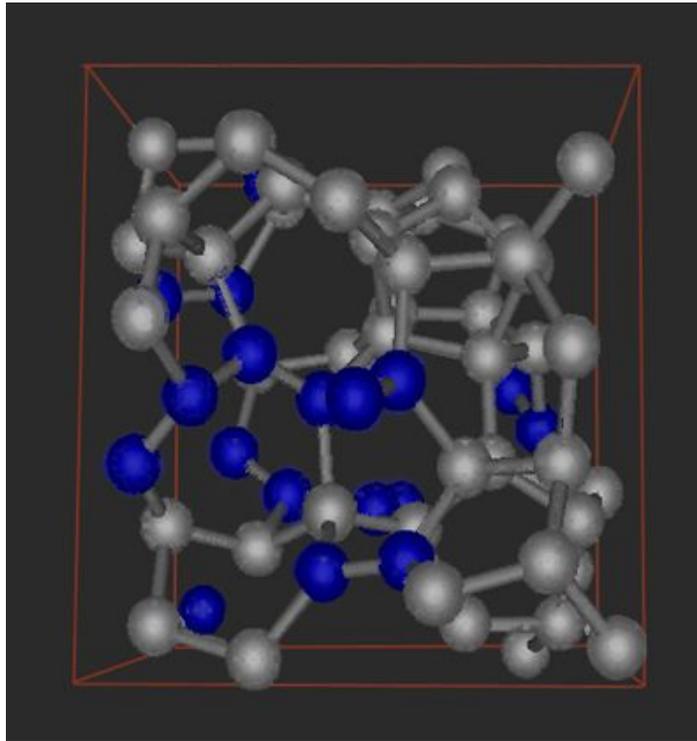
Tailoring materials for the future

Since the dawn of civilization, materials have been central to our growth, prosperity, security, and quality of life. Nevertheless, materials research as an identified field of



Sandia researcher Jeff Brinker observes the structures of a variety of submicroscopic spheres created by his team at the nanometer scale.

intellectual pursuit is less than 50 years old. Its emergence coincides with significant expansion of the field and its growing contributions to society.



Sandia has discovered a stress-free amorphous diamond thin film material that has many of the properties of crystalline diamond. The films as deposited have high stress, but a Sandia-discovered process allows for the complete tailoring of the final film stress state, from highly compressive through zero stress to tensile, depending on the need. The absence of film stress eliminates the old problem with film de-adherence and now enables thick coatings to be applied to components to impart wear-resistance and hardness.

New materials, or ways to make materials, are gaining greater use because of their improved properties. These properties result from the materials' composition and structure at all levels, down to their atomic or molecular structure and arrangement.

The field of materials research is defined by the strong interrelationships among materials' properties, structure and composition, synthesis and processing, and performance. In developing new materials, discovery and application, and therefore science and engineering, are closely interrelated.

Materials researchers study the structure and composition of materials on scales ranging from the electronic and atomic through the microscopic to the macroscopic. They develop new materials, improve established materials, and formulate methods to

produce materials reliably and economically. Researchers seek to understand phenomena and to measure materials properties of all kinds. They also predict and evaluate the performance of materials as structural or functional elements in engineering systems. This diversity of interests is reflected in the fields of materials researchers, who represent a broad range of academic departments and disciplines.

Materials researchers are found throughout industry, academia, and government. Their work can be limited to one or two researchers at a small

start-up company or may involve several hundred staff at a major materials research center such as Sandia. [See *PETL Facility*, page 14] Materials research also is an international endeavor. The Materials Research Society, one of the major professional societies in the field, has members from more than 60 countries.

Without new materials and their additional capabilities, many of the things that we take for granted at the dawn of the 21st century—modern cars and airplanes, telecommunications, medicine, and computers—could not exist.



Ron Brightwell examines the motherboard of one of Sandia's Cplant (Computational plant) computers. Cplant integrates hundreds of off-the-shelf computers and ranks among the world's fastest computers.

Sandia research has practical applications

Sandia's materials science and technology (MS&T) organizations undertake key research that forms the scientific basis for sound technical decisions about materials used in non-nuclear components for the nuclear weapons stockpile. These decisions range from materials choices, to the means of manufacturing components and estimating component lifetimes. MS&T staff research the synthesis and processing of materials and methods to determine their resulting structure, properties, and performance. Staff apply insights gained from these activities to studies of materials properties that have technological importance. Sandia's three major themes of materials research are *scientifically tailored materials, materials processing, and materials aging and reliability.*

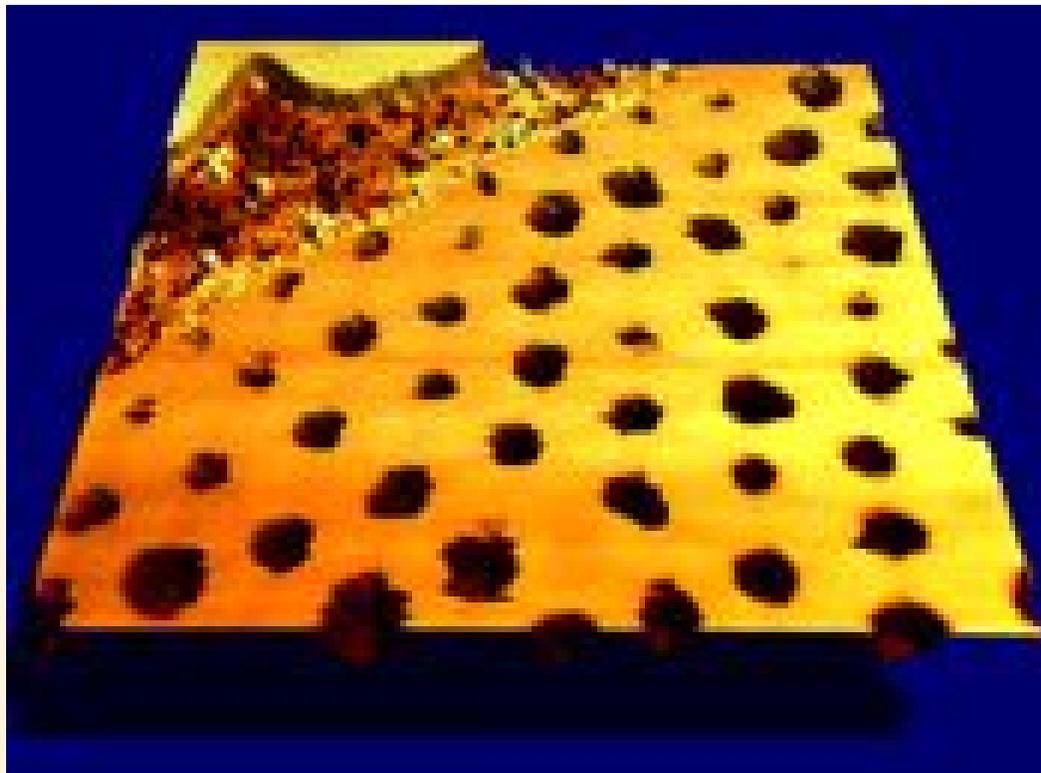
Without new materials and their additional capabilities, many of the things that we take for granted at the dawn of the 21st century—modern cars and airplanes, telecommunications, medicine, and computers—could not exist.

Our work in **scientifically tailored materials** addresses the need for materials with specific properties or performance characteristics. Projects emphasize achieving scientific understanding of how the materials properties depend on composition, microstructure, and preparation conditions. We use this understanding

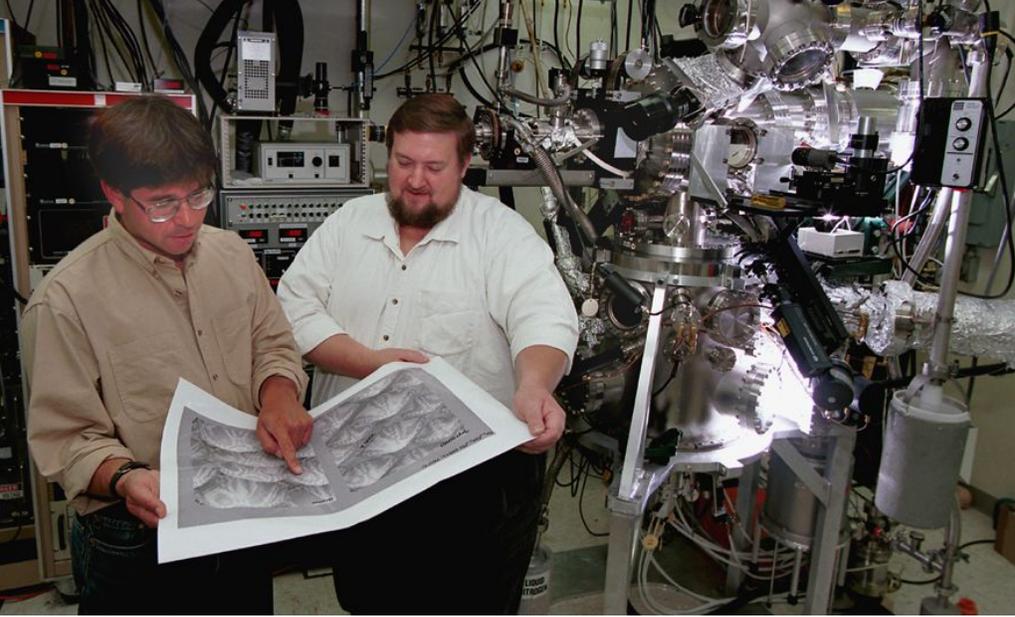
to develop materials with new properties or combinations of properties. This capability allows us to identify replacements for materials in the stockpile that are no longer available. We also develop new materials that simplify production, improve performance, or increase reliability and surety. [See *Affordable Hydrogen Getter*, page 11]

The **materials processing** effort develops a fundamental understanding of new and existing materials processing methods that are critical for defense and other needs. We are developing ways to fabricate parts faster, with fewer defects, and at lower cost. [See *Materials Researchers Bring Russian Cold Spray Technology to Sandia*, page 15]

Our effort in **materials aging and reliability** addresses the chemical and physical mechanisms that cause materials properties to change with time. We must understand important mechanisms involving both phenomena



This Swiss cheese-like micrograph shows the precision of a lacework pattern that emerges on a film of silver one atom thick and sprinkled with sulfur. The phenomenon is one of many that scientists witness as they study nanotechnology—the creation and manipulation of materials and devices built on a scale of nanometers. Scientists are studying what drives this process, which could enable new generations of revolutionary nanostructures or materials.



Sandia's Jerry Floro (left) and John Hunter examine an atomic force micrograph image of semiconductor quantum dots.

intrinsic to the materials themselves and those associated with the environments in which the materials are used. The scientific results from this work become the basis for quantitative predictions of component reliability over time in the stockpile. [See *One Wafer, Many Tests*, page 12] The methodology is equally applicable to materials reliability predictions in other high-consequence applications. [See *FAA Partnership*, page 8]

Modeling and simulation of materials and processes are critical to achieving advances in any of the three research areas. The people who develop and implement the models collaborate closely with the researchers who perform the experiments that validate the model results. Sandia has the expertise to simulate and predict the structures and properties of metal, ceramic, and polymer materials at length scales ranging from the macroscopic to atomic level. As we develop and validate materials models on some of the world's fastest computers, we are able to simulate the structures of surfaces, interfaces, and bulk materials; determine how the microscopic-scale structure of the material evolves during processing or use; and analyze materials properties and performance. [See *Solving a Mystery*, page 13]

New MESA Facility

Materials issues lie at the heart of MESA (Microsystems and Engineering Sciences Applications), a major new thrust at Sandia. MESA is a proposed state-of-the-art facility at Sandia National Laboratories that will provide the capabilities essential to maintain a safe, secure, and reliable stockpile. The facility will provide a single location for the design, integration, prototype fabrication, and qualification of integrated microsystems into weapon components, subsystems, and systems



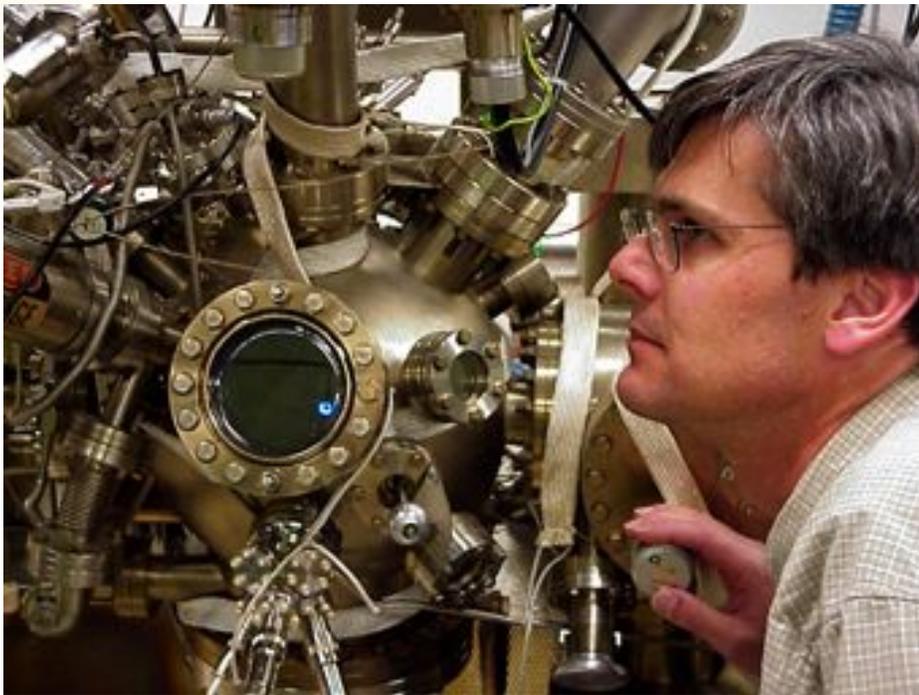
The proposed MESA facility at Sandia.

The materials-processing effort develops a fundamental understanding of new and existing materials processing methods that are critical for defense and other needs. We are developing ways to fabricate parts faster, with fewer defects, and at lower cost.

for the U.S. nuclear weapon stockpile.

Microsystems are not miniature versions of larger devices. Different physical mechanisms become important. For example, microsystems have a much higher percentage of atoms and molecules at surfaces and interfaces between materials than do larger devices. [See *New Materials for Microsystems*, page 7]

Materials research occurs at the interface between long-established fields, such as physics and chemistry. This inherent interdisciplinarity leads materials researchers to reach out to other fields in search of new connections and insights.



Materials scientists at Sandia are combining nanofabrication and surface characterization techniques to study the fundamental mechanisms of structural metal corrosion.

Researchers at Sandia are pursuing thrusts at two new interfaces that we expect to be very fruitful. The first stems from Sandia's cutting-edge work in multivariate analysis of spectral data. Recently, we have generalized and expanded these capabilities into the broader area of information discovery, extraction, and analysis (IDEA) of multivariate data from any source. This link to the information sciences is already being applied to materials analysis, biotechnology, satellite image analysis, seismic analysis, and process monitoring. [See *A Great IDEA*, page 9]

Another particularly successful area of research is at the interface between materials science and biology. Biological systems produce complex structures without a drawing of the final product. Instead, they self-assemble using information programmed into individual building blocks. The encoded information dictates structural patterns, hierarchy, length scales, function, response, and overall size by self-limiting. The end structure is typically an order of

magnitude or more larger than the individual components. Understanding the design rules for self-assembly should allow us not only to imitate some of the complexities of biological systems but also to intentionally design

Today's research will be the basis for new materials advances that will improve our lives for generations to come.

materials and materials systems of unheard of complexity on the nanoscale. [See *New Materials for Microsystems*, page 7]

Materials scientists and engineers at Sandia will continue to be at the forefront of these and other areas of science and engineering in the service of society as they achieve new levels of understanding and control of the basic building blocks of materials: atoms, molecules, crystals, and noncrystalline arrays. Today's research will be the basis for new materials advances that will improve our lives for generations to come.

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Pauline Ho at Sandia's Plasma Processing Research Lab, where plasmas, or hot gases, are used to clean the surfaces of weapon components to enhance adhesion. They also are used to etch circuits on microchips.

NEW MATERIALS *for Microsystems*

Microsystems—small devices that sense, think, and act—have been heralded as one of the major new technology revolutions. At Sandia, we view microsystems as one of the future's most important technologies, both for increased surety of weapon systems as well as for U.S. economic competitiveness.

Sandia is pursuing research and development to expand the range of materials available for application in microsystems to beyond just silicon. Extending the range of materials is particularly important for the sensing and acting elements of integrated microsystems. Sandia also is studying the material properties of silicon when it is used not just for integrated circuits, but in devices that are tiny, functioning machines.

Research in materials science to extend the materials choices for microsystems includes developing new processing techniques. A technique called LIGA, an acronym for the German words for lithography, electroplating, and molding, provides a platform for our research in microsystems materials. This technique relies on creating precise metal parts using X-ray synchrotron lithography and subsequent electroplating. The unique and rather valuable metal parts made using this technique can be used directly



Precision microcomponents fabricated with Sandia's LIGA technology.

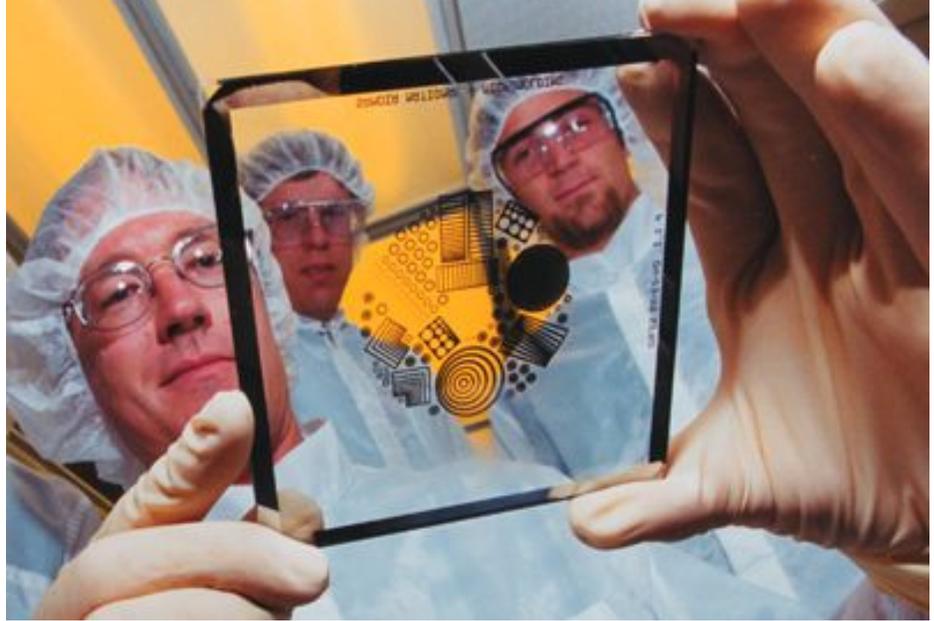
in applications, or the wafer full of metal structures can be used as a mold for replication. The most common method of replicating a metal master mold relies on an injection molding technique similar to the method used to make compact disks. The inexpensive plastic

replicates can then be used as individual plastic microparts, or alternatively the full wafer plastic replicate can be used again as a mold. The plastic mold can be filled with nanoparticles of ceramics, metals, or metal alloys that have unique properties. In a sense, this plastic mold can be thought of as a lost mold similar to that used in many macroscale materials processing technologies such as casting. Sandia has active programs in nanoparticle synthesis, LIGA processing, and microscale molding to explore this exciting area.

LIGA research and development is being extended to other processing techniques that also allow precision mold fabrication. Sandia researchers are developing new resists and materials that allow the use of thick ultraviolet processing and deep reactive ion etching to create more cost-effective molds or to further extend the capability of the process.

Research in materials science to extend the materials choices for microsystems includes developing new processing techniques. A technique called LIGA, an acronym for the German words for lithography, electroplating, and molding, provides a platform for our research in microsystems materials.

Sandia has licensed the LIGA-processing know-how to AXSUN Technologies, a U.S. telecommunications company. AXSUN is using LIGA metal microstructures in agile photonic subsystems (See *Sandia Technology Fall 2000, p. 12*). We are also working with several commercial partners interested in the technique for plastic and ceramic micropart fabrication.



Sandians Doug Chinn, Craig Henderson, and Michael Winter display a chrome mask for LIGA fabrication. Photo courtesy of East Bay (California) Business Times.

Other materials science initiatives that support microsystems development include:

- Manipulation of metal and silicon nanostructures and development of new diamond morphologies.
- Experimental and modeling efforts to assess the performance and reliability of materials interfaces.
- Exploratory science supporting future systems, namely nanosystems and molecular integrated microsystems.
- Studies on defect production and

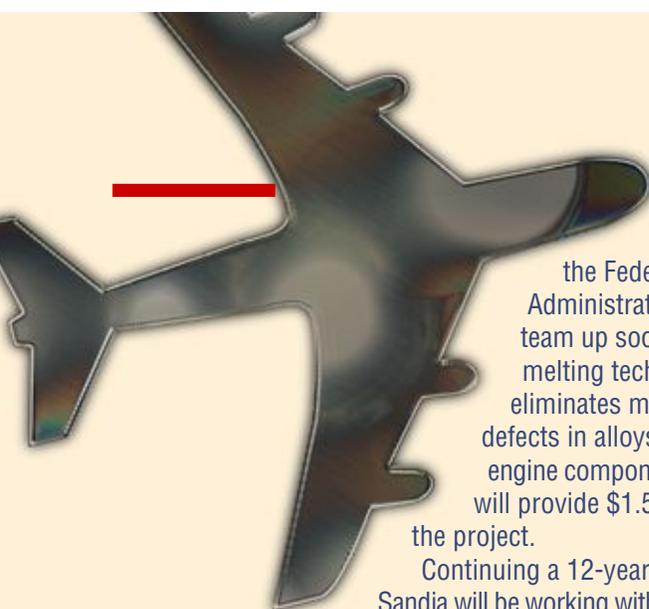
reduction in optical materials for advanced components and photosensitive materials for weak-link applications.

- Plasma-control research to support microelectronics fabrication and modeling.

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FAA Partnership to Reduce Alloy Defects



Sandia and the Federal Aviation Administration (FAA) will team up soon to research melting technology that eliminates melt-related defects in alloys for rotating engine components. The FAA will provide \$1.5 million for the project.

Continuing a 12-year partnership, Sandia will be working with the Specialty Metals Processing Consortium (SMPC). SMPC is a group of 13 U.S. specialty-metals producers and aerospace-alloy users collaborating to study specialty-metals production, processing, quality, and performance.

The partnership has developed expertise and a variety of resources including diagnostic tools, process models, advanced process controls, and melting facilities. These resources are available for research on defect reduction in alloys used for aircraft propulsion systems.

The FAA has recognized that an important asset of this partnership is the close working relationship Sandia has with the staff and management of member companies. This results in full communication of technical needs and ensures that new technology is rapidly incorporated into industrial practice.

Benefits to the Department of Energy include the application of melting science and technology to the melting of uranium alloys, and methods to decontaminate radioactive scrap-metal waste using liquid-metal processing.

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A Great IDEA for Materials Analysis

The Information Detection, Extraction, and Analysis (IDEA) program expands Sandia's capabilities in **multivariate analysis** (the study of random variables that are multi-dimensional). At the Materials and Process Sciences Center our expertise and facilities for infrared spectroscopy, mass spectroscopy, and chromatographic methods are combined with calibration and classification methods to solve problems surrounding materials analysis, aging, and characterization.

Multivariate analysis: Our calibration and classification capabilities can be applied to spectral data from mid- and near-infrared, visible, Raman, Auger, atomic emission, electron microscopy and ion mobility spectroscopies. We have improved quantitative and qualitative analyses and have developed new calibration methods for process monitoring and quality control.

In support of national security, our multivariate methods were developed to analyze seismic data to detect buried equipment, conduct remote satellite imaging, study the aging of nuclear weapons components, and ensure the nuclear weapons stockpile is safe, secure, and reliable.

We license software that has applications in process monitoring, materials aging, and noninvasive biomedical analysis and cell classification, as well as kinetics, corrosion, and quality control.

Hyperspectral imaging: A new FT-IR (Fourier Transform Infrared) spectrometer can generate detailed infrared hyperspectral images in minutes and provide them in a choice of macro- and microscopic scale. Algorithms can map the chemicals in samples. These



Sandia's Mike Sinclair (left) and Mike Butler prepare to put the dime-sized polychromator remote sensor chip into a testing unit.

tools can be applied to remote-sensing satellite imaging as well as to scanning-electron microscope imaging.

Weapon atmospheres:

Nuclear weapons surveillance requires sampling of the atmosphere inside the weapon and conducting quantitative analyses of these samples. The resulting data provide information on materials degradation and aging that may be occurring within the weapon. The normal gas composition (called the signature) of each weapon system is computed by combining new and existing methods. Resulting gas analyses are compared to the signature. Weapons with abnormal compositions are studied to determine the cause.

FT-ICR mass spectrometry:

This technology can measure mass precisely. (FT-ICR stands for Fourier Transform Ion Cyclotron Resonance.) It can distinguish between different elements by analyzing their mass. FT-ICR can also study ion-molecule reactions and kinetics.

Polychromator: A MEMS (microelectromechanical system)-based technology, the polychromator performs real-time detection and analysis of gases and does so safely from a remote location. The polychromator works by passing a sample gas through infrared radiation. The gas sample registers a spectral pattern. To identify the sample, its spectral pattern is then compared to the spectrum of a reference gas. Polychromator development is a joint effort with Sandia and the Massachusetts Institute of Technology designing the MEMS device, and Honeywell fabricating it. A prototype is expected this year.

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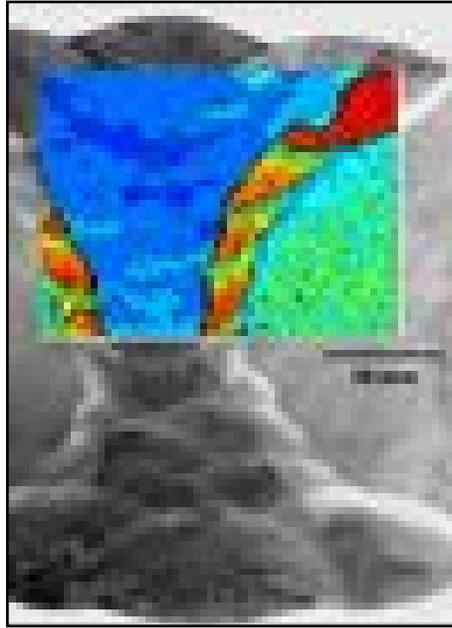


Sandia's materials and process computation and modeling effort develops computer models of materials and processes. These models help us understand the microstructures that link processing to performance. We study manufacturing process, materials aging, new-materials properties, and the effects of chemical and physical stresses.

Using mathematical models to predict materials behavior is called materials modeling. This method is expected to become an important tool for materials development and evaluation. Models range from simple to complex computer simulations.

During the past decade, materials modeling has become increasingly predictive. Previous materials modeling was qualitative. Advances in computing power and in computational algorithms have improved predictive capabilities. Useful across the spectrum of materials activities, this tool is part of a broader trend in science and engineering. Today, computer modeling and simulation supports most areas of scientific inquiry. Broad interest has developed in these methods, in part because fields outside of materials research have used these modeling capabilities successfully. An example is pharmaceutical design.

The challenge for materials modeling is to simulate and comprehend complexity. In recent years, materials researchers have used multi-scale modeling, an approach with a hierarchy of detail to describe materials. The coarsest level of modeling, used for engineering design, relies on knowledge gained from the finer-level models. Intermediate, or mesoscale, models simulate and predict structures and properties of materials, or the manner in which materials interface with other materials, how microstructures change



The hardness of a weld varies (false color) and can be related to the details of its microstructure.

Predictive Modeling Meets the Challenge of Understanding Complexity

during processing, and how these materials perform. Fine-scale models focus on the atomic-level behavior of individual defects. Scientists need to understand materials in more detail than the level at which they work. If they work on a macro-level, they need to understand materials properties at the micro-level. If they work at the micro-level, they need to understand properties at the nano-level.

The challenge for materials modeling is to simulate and comprehend complexity.

Materials modeling assists the three materials research areas at Sandia: materials processing, scientifically tailored materials, and materials aging-and-reliability studies.

For materials processing, researchers can create a detailed model of a process, then computer simulations can test the modification.

For scientifically tailored materials, modeling helps find materials with desired properties. Models provide insight into the origins of desired properties and provide a basis to suggest advantageous modifications. Computer simulations can "test" these modifications before the fabrication process, thus often saving time and money.

For materials-aging studies, computer models are required to find out how long a part will last. In accelerated-aging experiments, the researcher places the material in an environment, such as an elevated temperature that ages the part. However, a model is needed to compare the failure time under the accelerated conditions to the failure time under service conditions. The better the model is, the more accurate the predictions of materials aging and reliability are.

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Sandia's patented hydrogen-getter material can be processed into a variety of forms so it can be used as a powder, a pellet, an adhesive, or a coating. The rubbery polymer is similar to what you might find in a tire, says co-inventor Tim Shepodd.

Affordable Hydrogen Getter

Gets Good Marks

New patented hydrogen getters are made from commercial chemicals that are nontoxic and can be recycled so precious metals can be reclaimed. The new getters use polymers with double bonds that act like chemical hooks to catch hydrogen atoms. The new getter can be used in various applications, and has been commercialized for industrial use. It lengthens the life of heat exchangers (installations as big as buildings), maintains a vacuum for insulation, and is used in chemical processing.

Hydrogen build-up inside sealed chambers of the heat exchanger prevents correct operation. The hydrogen getters remove the hydrogen and the problem.

"This allows heat exchangers to last years longer," said Sandian Tim Shepodd.

Power plants and chemical refineries around the world now use hydrogen getters based on the Sandia design.

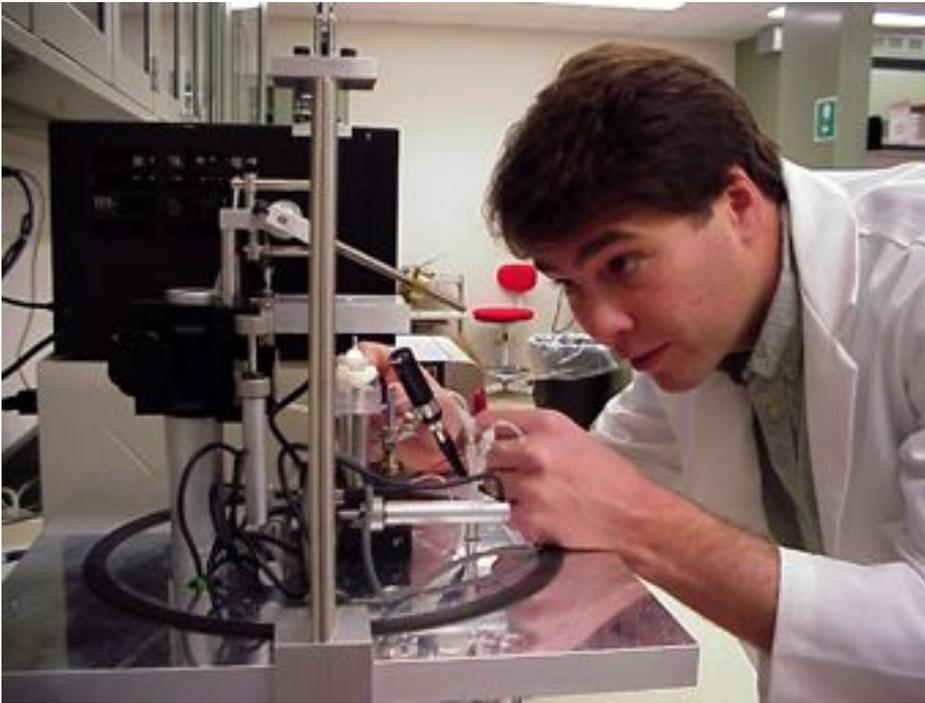
A patented spin-off technology removes explosive hydrogen build-up

in sealed consumer products powered by batteries.

"In a waterproof radio (for example) that could detonate and blow your hand off, we can bring hydrogen down to a safe level," Shepodd said.

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Initiation of localized corrosion in aluminum is being studied with a novel microelectrochemical cell. Nano-engineering techniques are used to control the aluminum microstructure and concentration of defects.

One Wafer, *Many Tests*

Atmospheric corrosion can be the bane of electronic performance. Copper, a conductor, is a key material used in electronics.

Corrosion can cause a component to fail. Understanding how corrosion occurs helps researchers to prevent it and predict the lifespan of electronic components. Sandia's Laboratory Directed Research and Development (LDRD) program has provided funds to develop analytical tools that predict corrosion behavior on both copper and aluminum.

Several Sandians are using LDRD funds to study how and why copper corrodes. Charles Barbour and Jeff Braithwaite are combining multiple

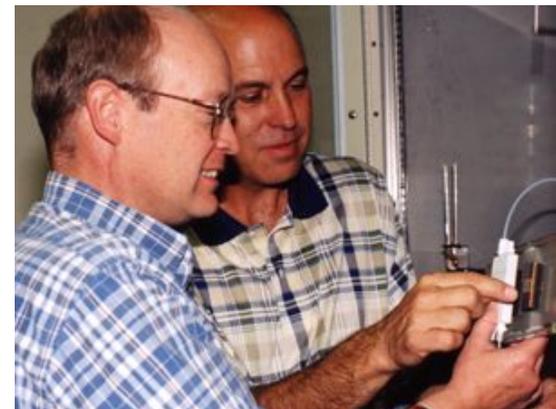
corrosion experiments on a single silicon wafer. This microlaboratory, called combinatorial experimentation, ensures all experiments are run simultaneously under identical conditions. This eliminates the problem of trying to reproduce the experiment. Used in biomedical research, the method is new to corrosion studies.

"In the past when we did copper corrosion tests," Barbour said, "we would put a piece of copper in an atmospheric chamber, add contaminants at very low levels, and run the experiment. But this serial approach is very time-intensive, and we were unsure that the environment was the

same experiment to experiment. It was difficult to compare results."

In one kind of combinatorial experiment, researchers used an electron beam to evaporate a thin copper film onto silicon wafers. Then portions of film were etched using photolithography and leaving thin, meandering lines of copper. The lines formed electrical resistors to monitor the extent of corrosion as a function of time. Impurities were implanted in the resistors. While the wafer was exposed to hydrogen sulfide, researchers used the change in resistance to calculate the copper-sulfide corrosion thickness on the meander lines. The study showed that indium slows corrosion, but deuterium accelerates it.

"These experiments show it's possible to use microcombinatorial techniques to efficiently characterize copper corrosion," said Jeff Braithwaite. "The small samples proved beneficial because the extent of corrosion could be easily monitored as a function of time and because all the experiments could be simultaneously performed."



Charles Barbour (left) and Jeff Braithwaite prepare a combinatorial experiment.

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Solving a Mystery Could Lead to New Material Properties

A Sandia materials researcher has solved a century-old mystery surrounding a type of metal that doesn't expand when heated. Known as *invar*, shorthand for *temperature invariant*, these few materials have physical properties that do not change with temperature variations.

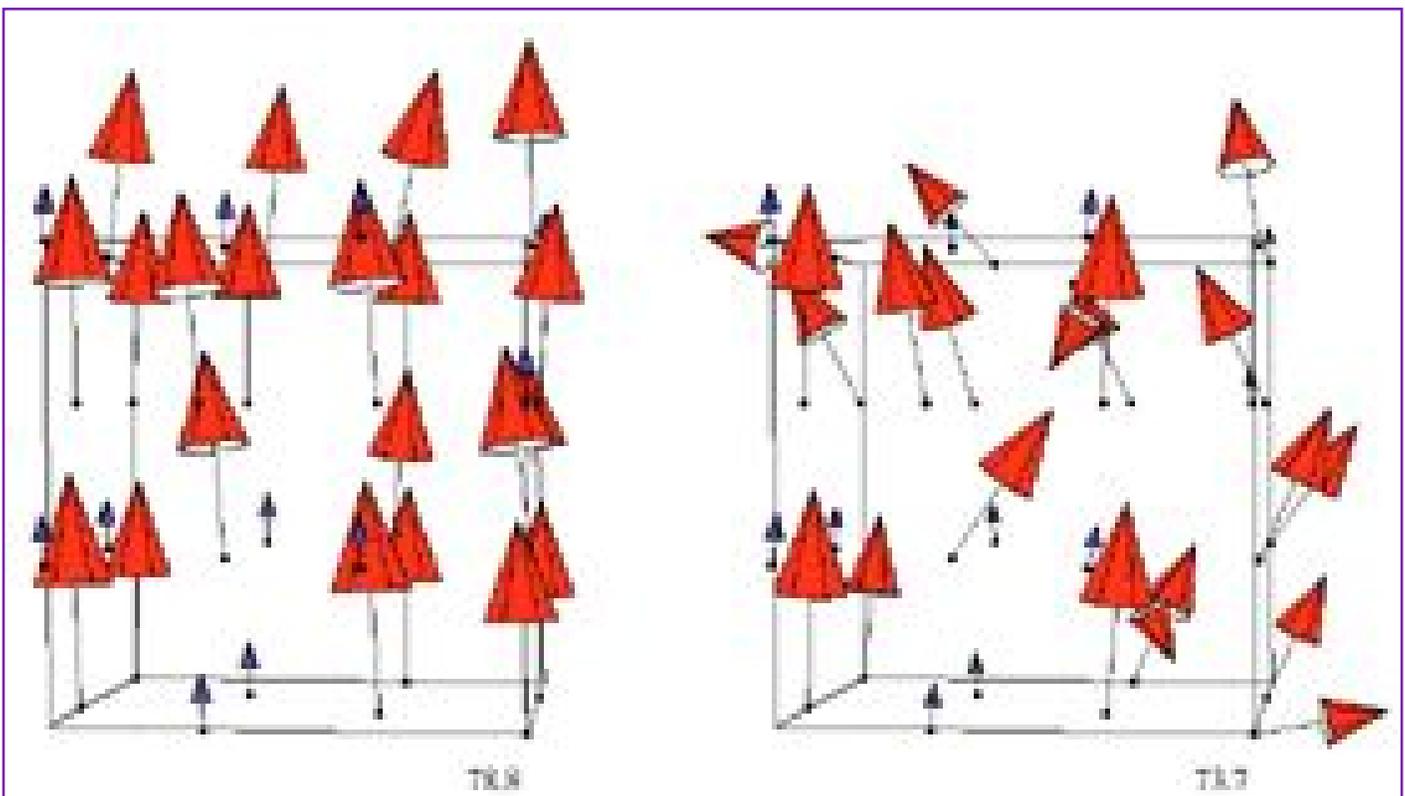
This is unusual because nearly all solids, liquids, and gases expand when heated. A hot can of soda pop is a good example. When heated, atoms jostle

about and push other atoms away more aggressively. In a typical solid, the individual atoms are constrained from moving too much because the forces that pin the atoms to their crystalline positions are strong. (This is why the expansion in a solid is less dramatic than in a gas). Each individual atom moves back and forth around its equilibrium position (like a swinging pendulum). The restoring force lies in the attraction between the positively charged nuclei and the negatively charged electrons. This attraction causes the atoms to assemble into a solid in the first place.

At very low temperatures the vibrations have small amplitude, and

the motion is symmetric around the center. At higher temperatures, the vibrations become increasingly asymmetric because the restoring force is weaker when the atoms are farther apart. Thus each atom spends slightly more time farther away from its neighbors than close to them.

However, *invar* is different. The restoring forces remain symmetrical, so the atoms maintain a symmetrical motion around the center. The cause was thought to be some anomalous property of the electronic structure. Scientists have known that *invar* is correlated with magnetism, but the precise mechanism has eluded description.



Calculated magnetic spin configurations of atoms in an iron-nickel *invar* alloy at two different volumes. Red and blue arrows show the magnetic moments on iron and nickel atoms, respectively. The sizes of the arrows indicate the size of the local magnetic moment. The spins of the nickel atoms are always oriented in the same direction (vertically in the figure), while the orientation of the spins of the iron atoms varies.

Usually magnetic atoms in a material align themselves in parallel, like trees growing upward in a forest. Temperature causes the atoms to gyrate somewhat, analogous to the wind causing the trees to sway.

Sandian Mark van Schilfgaarde who co-authored the cover story in *Nature*, July 1999, showed that an iron-nickel alloy (the first and best-known invar material) underwent a transition to a curious noncollinear state. (This means the tiny, atom-sized spins do not align parallel to one another even in their equilibrium state at low temperature.)

Usually magnetic atoms in a material align themselves in parallel, like trees growing upward in a forest. Temperature causes the atoms to gyrate somewhat, analogous to the wind causing the trees to sway. But with invar, van Schilfgaarde found that the magnetic spins behave differently. Nickel and iron spins tend to align with each other in the usual way, and similarly nickel atoms align with other nickel atoms. But iron atoms try not to align with other iron atoms. Thus begins a curious dance where the iron atoms try to align with nickel while at the same time trying to avoid one another. This unusual magnetic state alters the electronic restoring force and nearly cancels (or even reverses slightly) the asymmetry in the restoring force. This observation explains why invar does not significantly change properties when heated. Indeed, if the reversal could be enhanced, it could be possible to have a material that contracts as it is heated.

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Sandia's PETL Facility: Where Materials Science Happens

Sandia's Materials and Process Sciences Center has opened a \$45.9 million Processing and Environmental Technology Laboratory (PETL).

Research at the facility reinforces Sandia's mission of nuclear stockpile stewardship. The lab opened last summer and was dedicated in November. Materials-science research conducted at PETL supports nuclear weapons design, manufacture, surveillance, maintenance, and dismantlement.

Designed for teamwork and creativity, the 151,000-square foot facility offers new labs for aging and reliability studies, for developing scientifically tailored materials, process exploration, materials characterization, and modeling. To support research at the nanoscale, the building has floors that eliminate vibration. To ensure safe working conditions, the layout separates workers from chemicals, and air is not recirculated. The PETL building has two video conference rooms, seating areas for informal gatherings, small conference rooms, and a multipurpose room.

"PETL is an extraordinary resource that provides new opportunities for Sandians to exercise creativity," said Director Kay Hays of the Materials and Process Sciences Center.

The building offers plenty of natural lighting and easy access to staff and managerial offices.

"What's essential in our work is not just good research, but creativity," said Deputy Director Jim Jellison.

The PETL project won a Program and Project Management Award 2000 from the Department of Energy, the 1999 Excellence in Concrete Award (from the New Mexico chapter of the American Concrete Institute) for its structure and precast exterior, and the Energy Project of the Year (from the New Mexico chapter of the Association of Energy Engineers) for the chilled water thermal-energy storage system.



Materials Researchers Bring Russian Cold Spray Technology to Sandia

Cold-spray technology is one method of coating a surface to enhance wear and corrosion resistance. The cold-spray technique accelerates solid powder particles, which are at or near room temperature, to velocities of 500 to 1500 meters per second in a supersonic gas jet. The particles deform on impact and bond with the underlying surface.

The process compares to explosive welding on a much smaller scale. Cold spray can deposit metals and other ductile materials at a high rate. Steel and other alloys can be sprayed onto aluminum or other low-melting materials to increase hardness and wear resistance. Copper, aluminum, and other reactive metals can be cold-sprayed in open air with little or no oxidation. Cold spraying produces a higher thermal and electrical conductivity than traditional thermal spraying.

Developed in the Former Soviet Union, cold-spray technology was transferred to the United States by Sandia's Materials and Process Sciences staff, who then created a 10-member industrial consortium to research and commercialize this technology.

The cold spray initiative is a new part of the spray-coatings program, which includes thermal sprays. Some program accomplishments include:

- Development by Sandia and General Motors of a wear-resistant sprayed coating for cylinder walls in aluminum engines and a new process-control system for high-volume, highly reliable automotive spray coating. The resulting process diagnostics and modeling doubled production throughput and cut equipment costs by 50-percent.

- Development—with the Institute of Paper Science and Technology plus Thermal Spray Technologies—of an energy-management coating to foster a new papermaking process that uses 30-percent less energy than standard methods.
- Restoration of a scrap satellite part (worth \$150,000) using cold-spray deposition.
- Construction of a production spray-process control system to monitor and control velocity and temperature of the spray.

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Polymer Gels are Being Developed for Use as Actuators on a Microscale

Integrated microsystems for defense, for chemical sensing, and for medical applications of the future will rely on fast, efficient microactuators (small mechanical devices that respond to electrical signals) to serve as valves and pumps.

Sandia's μ ChemLab™ on a chip is an example of analytical equipment that is scaled down in size. A microlaboratory mounted on a computer chip, μ ChemLab™ can detect and analyze chemicals. Correspondingly small micromechanical structures, such as pumps and valves, must be developed. However, conventionally engineered mechanisms, such as electromechanical actuators, often cannot be scaled down and still function acceptably. Conductive polymer gels show

promise for microactuation because they use motion on a molecular scale to generate a macroscopic response (valve closure, for example).

Conductive polymer gels expand and contract when exposed to a small electrical stimulation. This dimensional change results from the diffusion of ions and electrolyte moving into or out of the gel. Pressure resulting from this inflow/outflow provides the activating force that could drive a valve, while the expansion and contraction can be used to pump fluids.

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INSIGHTS

by V.S. Arunachalam

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Materials Challenges for the Next Century

By V. S. Arunachalam

The cliché "we live in a material world" seems so true. Even a cursory cataloguing of materials around us adds up to an impressive list. There are so many to choose from—and almost all of them new—that we now enjoy the luxury of choice, a privilege denied to our ancestors. More materials have come into being in this century than all past centuries combined. Michael Ashby,* in one of his schematic diagrams, elegantly depicts the road traveled: from stones, flints, and pottery to tough engineering ceramics; from wood, skins, and fibers to polymers and plastics; from alluvial gold and copper to compound semiconductors. The list is truly grand.

History signposts periods of human achievement by the materials that made them possible: *neolithic*, to remind us of artisans who molded clay to pottery; and *chalcolithic*, when metals were smelted and shaped. The Bronze Age. The Iron Age. And thus the list goes on. What materials should represent this century? The sheer number of possibilities and lack of a historical distance make this a difficult choice. The spectacular growth of materials science and technology in this century has made its impact on materials development. Scientific rigor and technological competence have transformed the profession to become more deliberate and purposeful. The hunter has become the tiller.

As overtures for the next millennium begin to sound, we are tempted to speculate on materials that will persevere into the coming decades and beyond. In the midst of our discoveries, it was comforting to imagine that research and development determined the materials, the products, and even the market. But we now know that, more than ever, the market determines what the products will be. Good materials have floundered when there has been no market for them. The economist Joseph Schumpeter's argument that societal demands drive development and even research, is seen to be true in practically every example of technology. But for the market's demands for faster air travel—freeing one from long, turbulent, and claustrophobic intercontinental journeys—and faster and more agile military fighters, there would have been no jet engines or high-temperature superalloys. It is therefore prudent to speculate on what our society's longings are, and whether they are realizable at

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all with our current repertoire of knowledge and the materials required for the short term and for the decades beyond our current horizon. The need for new materials will emerge from such projections.

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* See M.F. Ashby, *Phil. Trans. R. Soc. Lond. A* 322 (1987) p. 393.

“As overtures for the next millennium begin to sound, we are tempted to speculate on materials that will persevere into the coming decades and beyond.”

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